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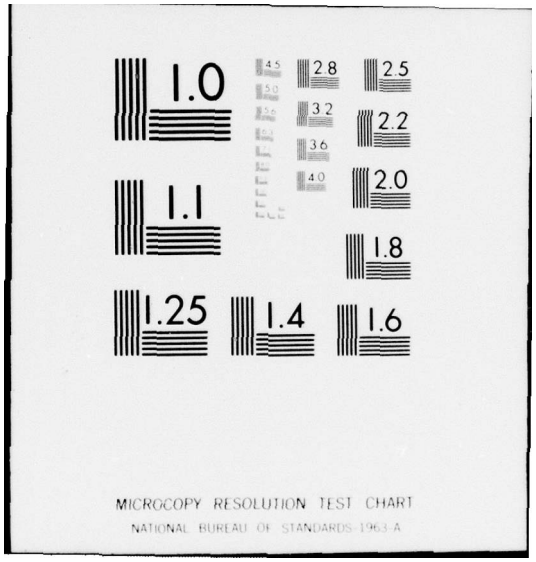
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ELECTRONIC EXCITATION IN NO AND SN BY THE NON-MUFFIN-TIN X-ALPHA METHOD

Douglas A. Ringers

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Theoretical investigations of the electronic structure of SN, of interest because of the explosive nature of $(SN)_x$, and its oxygen analogue NO, itself an important reaction product, have been performed by the x-alpha method using a perturbation technique to account for non-muffin-tin components of the charge density. The results, which differ from previous x-alpha calculations using overlapping sphere approximations to the charge density, are in good agreement with experimental values.

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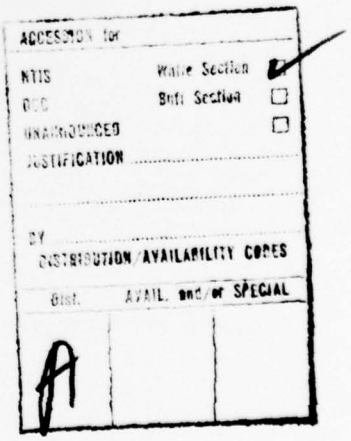

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I. INTRODUCTION

Nitrogen oxide (NO) is an important product of many gas-phase reactions involving propellants and explosives such as RDX and HMX, as well as chemiluminescent reactions. The compound is corrosive to metals and has a toxic effect on animal organs. These factors combine to make a study of NO relevant from many viewpoints.

The polymer sulfur nitride $(SN)_x$ has recently been the subject of many investigations, both experimental and theoretical, and may have unique military applications since, in addition to being an explosive[1], it is a one-dimensional conductor at room temperature down to a few degrees Kelvin. Unlike other one-dimensional metallic chains there is no metal-insulator transition[2]. In fact, at temperatures below .26°K, $(SN)_x$ becomes superconducting[3]. The sulfur nitride dimer S_2N_2 is also an explosive at room temperatures, and its monomer SN is the sulfur analog of nitric oxide.

The interest in these two compounds, coupled with the emergence of the Xα non-muffin-tin (NMT) codes[4], has prompted an investigation into electronic excitations of the two diatomics. The ionization potentials of the valence electrons of NO are relatively well known, while those of $(SN)_x$ have been less studied. The application of the Xα NMT codes should then be a test of the method for NO and a means of examining SN in its relation to NO, its oxygen analog.

II. THEORY

Electronic structure calculations were performed using the self-consistent-field X-α theory. The Xα method has been described in detail elsewhere[5]. It is necessary here to mention only some of its salient features. The feature that distinguishes the Xα method from a Hartree-Fock (HF) method, and upon which would depend its advantages, is the adoption of a local density approximation to the exchange-correlation

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1. J. Sharma, Private Communication.
2. V.T. Rajan and L.M. Falicov, Phys. Rev. B 12, 1240 (1975).
3. R.L. Greene, G.B. Street, L.J. Secter, Phys. Rev. Lett. 34, 577 (1975).
4. J.B. Danese, J. Chem. Phys. 61, 3071 (1974).
5. J.C. Slater, Quantum Theory of Molecules and Solids, Vol. IV, McGraw-Hill, New York 1974.

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term. This term, dependent upon the variable r, is usually written

$$U_{X\alpha\uparrow}^{(1)} = - 9\alpha \left\{ (3/4\ \pi)\rho(\vec{r}) \right\}^{1/3} , \qquad (1)$$

where ρ is the charge density given by

$$\rho(1) = \sum_i n_i\ u_i^*(1)u_i(1) , \qquad (2)$$

the u_i are/spin orbitals, and n_i is the occupation of the $i^{\underline{th}}$ spin orbital.

This term (1) replaces the usual HF exchange-correlation term,

$$\sum_j \delta(m_{s_i}, m_{s_j}) \int u^*_i\ (1)\ u^*_j\ (2)\ \frac{1}{r_{12}}\ u_j(1)u_i(2)dv_2/u^*_i(1)u_i(1).$$

The integration over pairs of coordinates will obviously make it a more time-consuming numerical process.

The Xα eigenfunctions and eigenvalues agree closely with results from HF methods for closed-shell atoms and with the Hyper-Hartree-Fock[6] method for open-shell atoms for suitable values of α.

The common procedure for applying the Xα method to molecules has used a muffin-tin (MT) approximation to the potential. In this approximation every atomic nucleus in a molecule is surrounded by a region of spherical charge density or potential. These spherical regions of potential were originally taken to be non-overlapping, and the potential between these atomic spheres was taken to be a constant. This approximation was found to work well for largely ionic molecules and solids. Good results were obtained for electronic excitations, values of the crystal field parameter, and even estimates of the interatomic exchange integral[7].

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6. J.C. Slater, J.B. Mann, T.M. Wilson, and J.H. Wood, Phys. Rev. 184, 672 (1969).
7. D.A. Ringers, A "First Principles" Calculation of the Heisenberg Exchange Intergral and Crystal Field Parameter for Nickel Oxide, Ph.D. Thesis, Univ. of Fla., Gainesville, Fl, 1973 (unpublished).

The calculation of electronic excitations and total energies for some less ionic compounds, as well as for many diatomic molecules, led to erroneous results. Some results were so in error as to predict that many known diatomic compounds would not even exist, that is, the atoms would not be bound so as to form a molecule[8].

Work to circumvent this shortcoming proceeded along two different approaches. One approach was to allow the atomic spheres to overlap. It was found that improved agreement with experimental values resulted, although no theoretical justification for the amount of overlap usually required was provided[9]. This approach led to the inclusion of "empty" spheres[10], regions of spherically averaged potential centered at other than atomic nuclei. It was then found that with enough empty spheres, whose radii and centers could be determined as necessary, and with overlapping atomic spheres whose radii were treated as adjustable parameters good agreement with experiment could often be obtained. Unfortunately, there is no theoretical means of establishing radii for empty spheres, although a rule of thumb for atomic spheres did develop[11]. This state of affairs could lead to making many calculations in order to obtain the "best fit" to experiment.

The other approach was to do away with the muffin-tin approximation, long thought to be the largest source of error. Ellis and coworkers[12] developed an Xα discrete variational method which does not rely upon the muffin-tin approximation to the potential but instead calculates the actual Xα potential. Danese, then at the University of Florida, developed a formalism for calculating not the actual Xα potential directly, but for calculating the difference between the Xα potential and its muffin-tin approximation by a procedure analogous to a perturbation technique. This non-muffin-tin (NMT) correction includes terms proportional to a charge density (the first order or linear terms) and terms proportional

8. E.C. Linsenmeyer, Diatomic Potential Curves by the Multiple Scattering X-Alpha Method, Thesis, Univ. of Fla., Gainesville, Fla., 1974 (unpublished).
9. F. Herman, A.R. Williams, and K.H. Johnson, J. Chem. Phys. 61, 3508 (1974).
10. K.H. Johnson, F. Herman and R. Kjellander, Applications of the SCF X-α Scattered-Wave Method to Molecules Crystals and Polymers, P. 601 in "Electronic Structure of Polymers and Molecular Crystals", Plenum, New York, 1975.
11. J.G. Norman, J. Chem. Phys. 61, 4630 (1974).
12. T. Parameswaran and D.E. Ellis, J. Chem. Phys. 58, 2088 (1973).

to a product of charge densities (the second order terms). It may be expressed as[4]

$$\Delta E(L) = \int \Delta\rho(\vec{r})\,\Delta V_{ne}(\vec{r})\,d\vec{r} + \int \Delta\rho(\vec{r})\,\Delta V_{c}((\bar{\rho}),\vec{r})\,d\vec{r}$$
$$+ c_{\alpha\uparrow}\int\left\{\rho_{\uparrow}(\vec{r})^{4/3} - \left[\bar{\rho}_{\uparrow}(\vec{r})\right]^{4/3}\right\}d\vec{r}$$
$$+ c_{\alpha\downarrow}\int\left\{\rho_{\downarrow}(\vec{r})^{4/3} - \left[\bar{\rho}_{\downarrow}(\vec{r})\right]^{4/3}\right\}d\vec{r} \qquad (3)$$

$$\Delta E(so) = \iint \frac{\Delta\rho(\vec{r})\,\Delta\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}\,d\vec{r}\,'\,d\vec{r} \quad . \qquad (4)$$

III. RESULTS AND DISCUSSION

The muffin-tin approximation (MT) to the potential was used, and the first-order correction terms for the difference between the actual X-alpha potential and the muffin-tin potential were calculated. In performing the MT calculations, the ratios of the atomic sphere radii were the same as those of the atomic radii given by Slater[13]. The NMT correction was calculated for small deviations from this prescription with the resulting total energy insensitive to these small variations. Since no overlapping, interstitial, or peripheral spheres are used in this method, no "calibrating" calculations were necessary to determine the non-atomic sphere radii. All states were allowed to adjust towards self-consistency during each iteration, and each excitation was calculated as a difference in total energies, so as to include orbital relaxation effects.

The values for alpha are those which approximately satisfy the virial theorem for the respective free atoms and a suitably chosen average over the non-atomic regions.

The free atom limits were obtained from those given by Schwarz[14], who used values of alpha leading to Hartree-Fock total energies, by the relationship

$$E_{X\alpha}(\alpha) = E_{HF}(\alpha_{HF}) - \Delta\alpha\,\frac{\partial E}{\partial\alpha} \quad ,$$

13. J.C. Slater, Quantum Theory of Molecules and Solids, Vol. II, McGraw-Hill, New York, 1965.
14. K.H. Schwarz, Phys. Rev. B 5, 2466 (1972).

where $E_{X\alpha}$ is the Xα total energy, dependent upon α; E_{HF} is the Hartree-Fock value of the total energy; α_{HF} is the α value leading to this energy; $\frac{\partial E}{\partial \alpha}$ is the energy dependence upon α and Δα is the difference between the α_{HF} obtained by Schwarz and the α values used in the present work. The relevant values are listed in Table I.

TABLE I. Xα Free Atom Limits.

Atom	$-E_{HF}$(ryd)[a]	α_{HF}	$-\frac{\partial E}{\partial \alpha}$	Δα	$-E_{X\alpha}$(ryd)
N	108.5923	.75197	17.2	.00245	108.550
O	149.5384	.74447	21.8	.00329	149.467
S	794.9572	.72475	69.0	.00292	794.756
Molecule					
NO					258.017
SN					903.306

[a] E_{HF}, α_{HF}, $\frac{\partial E}{\partial \alpha}$ as given in Ref. 14.

Experimental values of the internuclear separations[15,16] 2.1758 a.u. for NO and 2.8265 a.u. for SN, were used. Total-energy calculations were made for many different single-electron configurations of NO and SN. Those excitations leading to ionization are listed in Table II for NO and Table III for SN. In cases where a non-spin-polarized calculation does not lead to a unique transition, an average is given of the multiplets taken from the indicated reference, weighted according to their multiplicities. Calculated electronic transitions are given for NO in Table IV. The ionization potentials are shown in Figure I and Figure II for NO and SN, respectively.

15. G. Herzberg, Molecular Spectra and Molecular Structure I. Spectra of Diatomic Molecules, Van Nostrand, Princeton, 1950.

16. V.V. Walathka, M.M. Labes, and J.H. Perlstein, Phys. Rev. Lett., 31, 1139 (1973). M. Boudeulle and P. Michelle, Acta Crystallagr. A28, 5199 (1972).

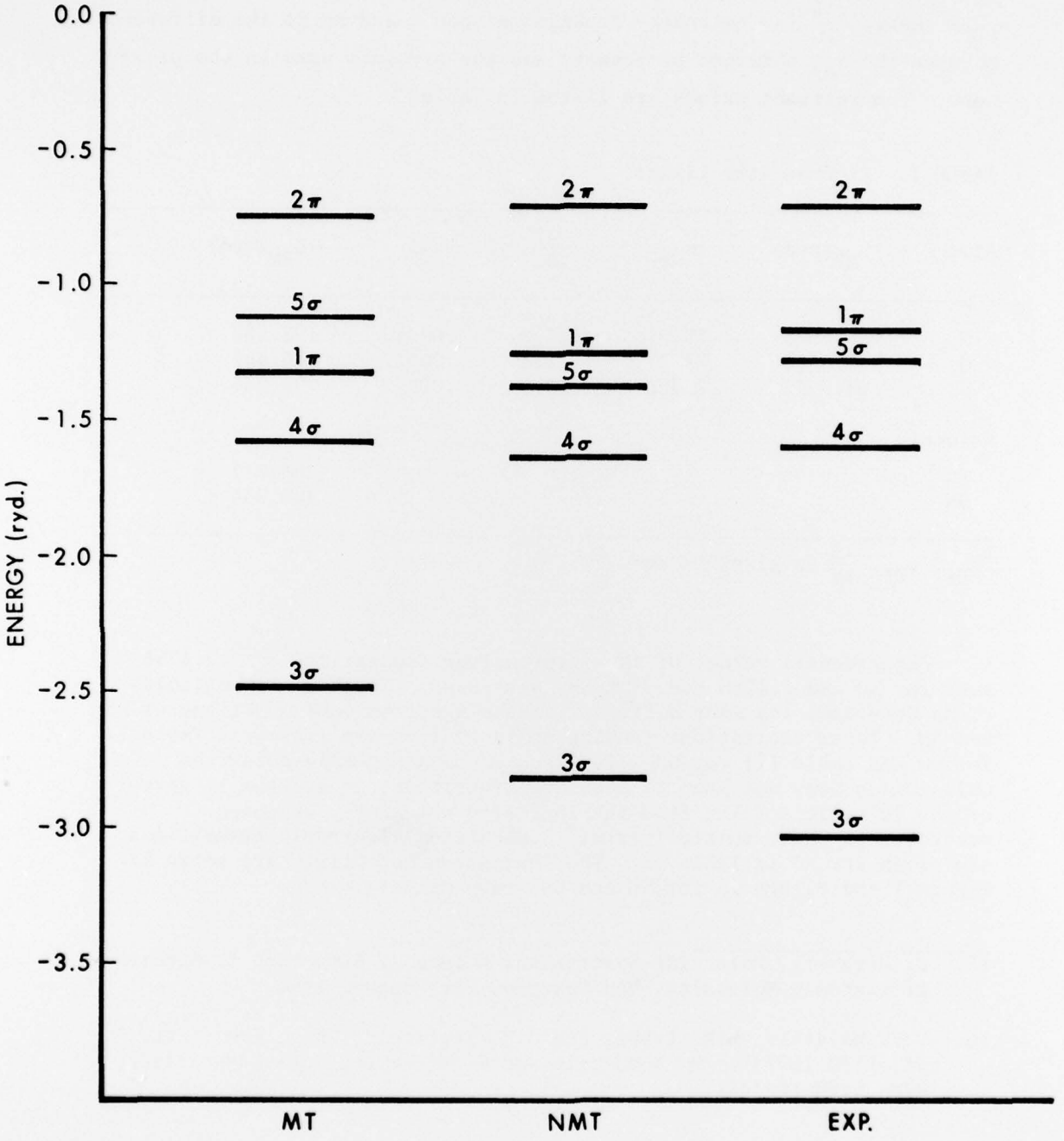

Figure 1. Ionization Spectra - NO

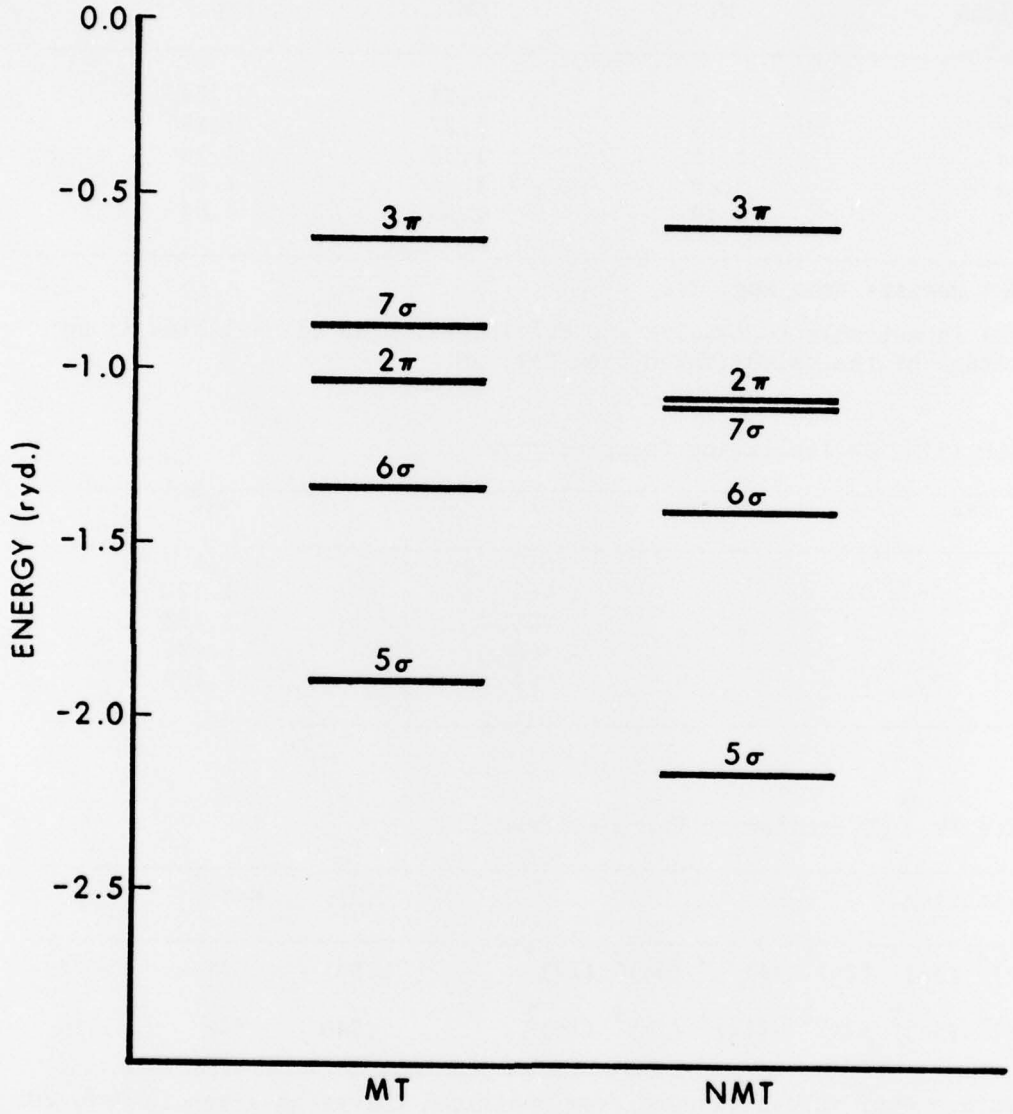

Figure 2. Ionization Spectra-SN

TABLE II. NO Ionization Energies (ryd.).

Orbital	MT	NMT	Exp.[a]
2π	.78	.74	.74[b]
1π	1.35	1.27	1.19
5σ	1.15	1.39	1.26
4σ	1.60	1.66	1.62
3σ	2.49	2.83	3.04

[a] ESCA results from Ref. 24.

[b] ESCA is not able to resolve the multiplets. The value listed is an average of the values taken from Ref. 20.

TABLE III. SN Ionization Energies (ryd.).

Orbital	MT	NMT
3π	.653	.624
2π	1.065	1.102
7σ	.905	1.128
6σ	1.365	1.428
5σ	1.911	2.179

TABLE IV. NO Excitation Energies (ryd.).

Excitation	MT	NMT	Exp[a]
$(1\pi)^4\ (3\sigma)^2\ (2\pi)^1 \rightarrow (1\pi)^3\ (3\sigma)^2\ (2\pi)^2$	.561	.538	.504
$(1\pi)^4\ (3\sigma)^2\ (2\pi)^2 \rightarrow (1\pi)^4\ (3\sigma)^1\ (2\pi)^2$	.340	.646	.628

[a] Average over values deduced from empirical curves as given in Ref. 20.

There are several interesting features to be noticed. In the MT calculations for both NO and SN, the results imply no binding of the molecule, whereas the NMT calculations predict binding. The NMT results give a binding energy for NO of .6 Ryd compared with an experimentally

inferred value of approximately .5 ryd.[17]. Inclusion of the second-order correction terms should account for much of the discrepancy between the calculated and experimental binding energies since the second-order terms may be as large as ten to twenty percent of the first order terms and are of opposite sign[18].

The relative ordering of the 1π and 5σ levels for the NMT calculation on NO agrees with that of several ab initio calculations[19,20]. It is in the same order as the 2π and 7σ orbitals in SN while it is the opposite of recently reported overlapping sphere Xα results[21] for NO.

The MT calculation for SN cannot distinguish between the ground state valence shell configuration $(7\sigma)^2\ (2\pi)^4\ (3\pi)^1\ (8\sigma)^0$ and $(7\sigma)^2\ (2\pi)^4\ (8\sigma)^1(3\pi)^0$ since they are of equal total energy. On the other hand, the NMT calculation selects the former configuration in agreement with previously reported calculations[17].

Table V lists the NMT contributions to the ground state energy and to the orbital energies of the valence electrons for NO and SN. We note that in every case the correction for SN is within 3 percent of that for NO, the maximum difference being only about 1 eV, whereas the total energies differ by over 645 ryd., a factor of nearly 3.5.

TABLE V. First-Order NMT Corrections (Ryd.)

State		NMT Correction		
NO	SN	NO	SN	Δ[a]
Ground State		2.848	2.772	.019
2π	3π	2.890	2.801	.031
1π	2π	2.897	2.824	.015
5σ	7σ	2.581	2.550	- .021
4σ	6σ	2.745	2.709	- .019
3σ	5σ	2.510	2.504	- .044

[a] Δ is 98% of the NMT value for NO minus the corresponding NMT value for SN.

17. A.G. O'Hare, J. Chem. Phys. 52, 2992 (1970).
18. J.B. Danese, to be published.
19. P. Siegbahn and H. Siegbahn (unpublished) cited in ref. 20.
20. H. Lefebvre-Brion and C.M. Moses, J. Chem. Phys. 44, 2951 (1966).
21. Dr. Salahub and R.P. Messmer, J. Chem. Phys. 64, 2039 (1976).

It may thus be that two different molecules comprised of atoms having correspondingly equivalent ground state valence shell structures will have nearly equal NMT corrections. If this should turn out to be the case, it would be necessary to calculate the NMT correction for only small appropriate molecules in order to obtain a very good estimate of the NMT correction for larger, more complex, molecules. If such a procedure had been adopted in the present work, using 98% of the NMT correction for NO as a suitable approximation of the NMT correction for SN, the maximum error would have been only about .6 eV. This conjecture remains to be proved and will require further investigation in order to test its validity.

The molecular crystal $(SN)_x$ is reported to have strong covalent bonds[22] in agreement with the present calculations which show the two highest π and the three highest σ states to be largely covalent. It has been reported that strong intrachain bonds are saturated with σ and π electrons, while the remaining electron, which results in the metallic behavior attributed to the material, has mixed σ and π character[22]. The present calculations indicate that energetically the residual electron has little preference for σ or π, with the π state having a slightly lower energy. Figure III shows, along with previously reported valence bands[23], the results of the present work. Good agreement was achieved, and calculations on increasingly larger clusters may be expected to show the evolution of the indicated single-electron eigenvalues into the energy bands shown.

Although the MT approximation does not indicate a bound molecule, many excitation energies agree well with experimental values. In such cases the error in the calculated total energy of the ground state and that of the excited state are nearly equal, so that a subtraction in order to obtain an excitation energy entails a large amount of error cancellation and yields reasonable results. Unfortunately, there is no way yet developed to determine when just such a cancellation will occur. In those cases where large error cancellation does occur, the error in the MT value is comparable to that of the first order NMT value. The circumstance of an error cancellation for some excitations and not for others may lead to an incorrect ordering of states. For example, in the present work, the 5σ state of NO is found to lie above its 1π state in the MT approximation with similar results occurring for the $7\ \sigma$ and $2\ \pi$ states of SN. The NMT calculations give the opposite ordering. Table II shows that the NMT values for these two states are

22. M. Schluter, J.R. Chelikowsky and M.L. Cohen, Phys. Rev. Lett. 35, 859 (1975).
23. D.E. Parry and J.M. Thomas, J. Phys. C 8, L45 (1975).

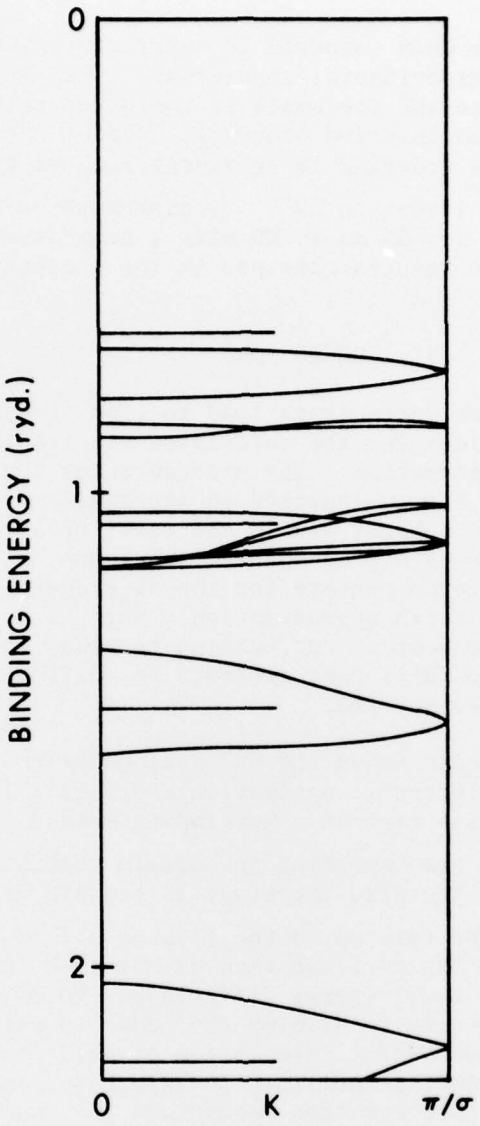

Figure 3. SN Valence Electron Energy Band Structure (Adapted from Reference 23) and Diatomic Eigenvalues.

both slightly too large when compared to experiment, but the separations are comparable to the experimental separation. The MT result, however, is too large in one case and too small in the other resulting in a much larger separation and an inverted ordering. Recent overlapping sphere MT calculations show an ordering in agreement with experiment for NO but show the two levels to invert in SN[21]. Recent Hartree-Fock calculations[18] show the same ordering for SN as in NO with a separation of .4 eV., in good agreement with the results obtained in the present NMT calculation.

IV. CONCLUSIONS

The NMT first order corrections lead to good agreement with previously reported values for the calculated electronic states and take about the time of one iteration. The procedure for the NMT total energy corrections is free of the ambiguities in the choice of number, size, and placement of non-atomic spheres and in the radii of atomic spheres, that are characteristic of overlapping sphere techniques. The first order corrections slightly overcompensate for the discrepancy between the $X\alpha$ potential and its muffin-tin approximation. Work is currently underway to incorporate the second order corrections to study their relative importance, and to allow different orbitals for different spins so as to better resolve multiplet spectra.

The calculations have shown the NMT X-alpha method to be a viable means of determining electronic excitation energies. This result is significant not only as a test of a developing method but also because electronic excitations are important in certain combustion processes[25]. Electronic excitations are also important in certain desorption phenomena[26] which may be related to the flaking off of scale in the erosion of gun tubes. The positive results obtained for the electronic excitations, which are total energy differences, in NO and SN indicate that it would be worthwhile to develop the means to calculate absolute total energies. The successful calculation of absolute total energies is critical in understanding chemisorption processes in gun tube erosion and in indicating possible reaction mechanisms in propellants and explosives. Efforts are currently underway to achieve this goal by extending the present work.

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25. L.E. Harris, "The Reactivity of Nitrate Esters", BRL R 1708, US Army Ballistic Research Laboratories, April 1974, (AD 919316L).
26. D. Menzel, in Interactions on Metal Surfaces, pp 102, Springer-Verlag, Berlin (1975).

REFERENCES

1. J. Sharma, Private Communication.

2. V.T. Rajan and L.M. Falicov, Phys. Rev. B12, 1240 (1975).

3. R.L. Greene, G.B. Street, L.J. Secter, Phys. Rev. Lett. 34, 577 (1975).

4. J.B. Danese, J. Chem. Phys. 61, 3071 (1974).

5. J.C. Slater, Quantum Theory of Molecules and Solids, Vol. IV, McGraw-Hill, New York 1974.

6. J.C. Slater, J.B. Mann, T.M. Wilson, and J.H. Wood, Phys. Rev. 184, 672 (1969).

7. D.A. Ringers, A "First Principles" Calculation of the Heisenberg Exchange Integral and Crystal Field Parameter for Nickel Oxide, Ph.D. Thesis, Univ. of Fla., Gainesville, Fla., 1973 (unpublished).

8. E.C. Linsenmeyer, Diatomic Potential Curves by the Multiple Scattering X-Alpha Method, Thesis, Univ of Fla., Gainesville, Fla., 1974 (unpublished).

9. F. Herman, A.R. Williams, and K.H. Johnson, J. Chem. Phys. 61, 3508 (1974).

10. K.H. Johnson, F. Herman and R. Kjellander, Applications of the SCF X-α Scattered-Wave Method to Molecular Crystals and Polymers, P. 601 in "Electronic Structure of Polymers and Molecular Crystals", Plenum, New York, 1935.

11. J.G. Norman, J. Chem. Phys. 61, 4630 (1974).

12. T. Parameswaran and D.E. Ellis, J. Chem. Phys. 58, 2088 (1973).

13. J.C. Slater, Quantum Theory of Molecules and Solids, Vol. II, McGraw-Hill, New York, 1965.

14. K.H. Schwarz, Phys. Rev. B 5, 2466 (1972).

15. G. Herzberg, Molecular Spectra and Molecular Structure I. Spectra of Diatomic Molecules, Van Nostrand, Princeton, 1950.

16. V.V. Walathka, M.M. Labes, and J.H. Perlstein, Phys. Rev., Lett. 31, 1139 (1973). M. Boudeulle and P. Michelle, Acta Crystallagr. A28, 5199 (1972).

17. A.G. O'Hare, J. Chem. Phys. 52, 2992 (1970).

18. J.B. Danese, to be published.

19. P. Siegbahn and H. Siegbahn (unpublished) cited in ref. 20.

20. H. Lefebvre-Brion and C.M. Moser, J. Chem. Phys. 44, 2951 (1966).

21. Dr. Salahub and R.P. Messmer, J. Chem. Phys. 64, 2039 (1976).

22. M. Schluter, J.R. Chelikowsky and M.L. Cohen, Phys. Rev. Lett. 35, 859 (1975).

23. D.E. Parry and J.M. Thomas, J. Phys. C 8, L45 (1975).

24. K. Siegbahn, et al., ESCA Applied to Free Molecules, North-Holland, Amsterdam (1971).

25. L.E. Harris, "The Reactivity of Nitrate Esters", BRL R 1708, US Army Ballistic Research Laboratories, April 1974, (AD 919316L).

26. D. Menzel, in Interactions on Metal Surfaces, pp 102, Springer-Verlag, Berlin (1975).

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